ECE 371
Materials and Devices

09/05/19 - Lecture 5

Infinite Potential Well and Step Potential Function (Part I)

General Information

- Homework #1 returned after class Tuesday. Solutions posted.
- Homework #2 assigned and due Thursday September 12th.
- Link to download Crystal Viewer (http://crystalmaker.com/crystalviewer/index.html) added to the website in Articles, Videos, and Additional Notes folder. See next few slides for examples of software capabilities.
- Reading for next time: 2.3.3-2.3.4

Schrodinger's Wave Equation

- The Schrodinger equation (SE) describes the spatial and temporal evolution of the wave function for a given potential energy landscape and set of boundary conditions

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = j\hbar\frac{\partial\psi(x,t)}{\partial t}}$$

related to kinetic energy | related to potential energy | related to total energy

- $V(x)$ is the potential energy, m is the mass of the particle, and $j = \sqrt{-1}$
- SE is a basic postulate of quantum mechanics but can be derived
- SE can be used to describe the behavior of electrons in a crystal

Time-Dependent and Time-Independent Parts of SE

- The separation of variables technique can be used to deconstruct the SE into time-dependent and time-independent parts
- We assume that the wave function can be represented as the product of a time-independent function and a time-dependent function (i.e., $\psi(x,t) = \psi(x)\phi(t)$)

Time-dependent solution can be obtained quickly:

$$\boxed{\phi(t) = e^{-j\left(\frac{E}{\hbar}\right)t} = e^{-j\omega t}}$$

Sinusoidal variation with time

E is the total energy of the particle

KE PE

Time-independent part of the equation:

$$\boxed{\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\big(E - V(x)\big)\psi(x) = 0}$$

Nature of the solution for $\psi(x)$ depends upon the potential V(x) and the boundary conditions

*see in-class derivation

Electron in Free Space

When V(x) = 0 we have a free electron and the TISE becomes:

$$\boxed{\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0}$$

wave number:

$$\boxed{k = \sqrt{\frac{2mE}{\hbar^2}}}$$

relates to total energy

The general solution is two travelling waves:

$$\boxed{\psi(x,t) = A\,exp[j(kx - \omega t)] + B\,exp[-j(kx + \omega t)]}$$

For a travelling wave in the +x direction we have:

$$\boxed{\psi(x,t) = A\,exp[j(kx - \omega t)]}$$

- The probability density function is a constant (AA^*)
- Particle can be found anywhere since the momentum is well defined
- Note that the plane wave solution cannot be normalized (but a superposition of plane waves can be – wave packet)

Potential Wells

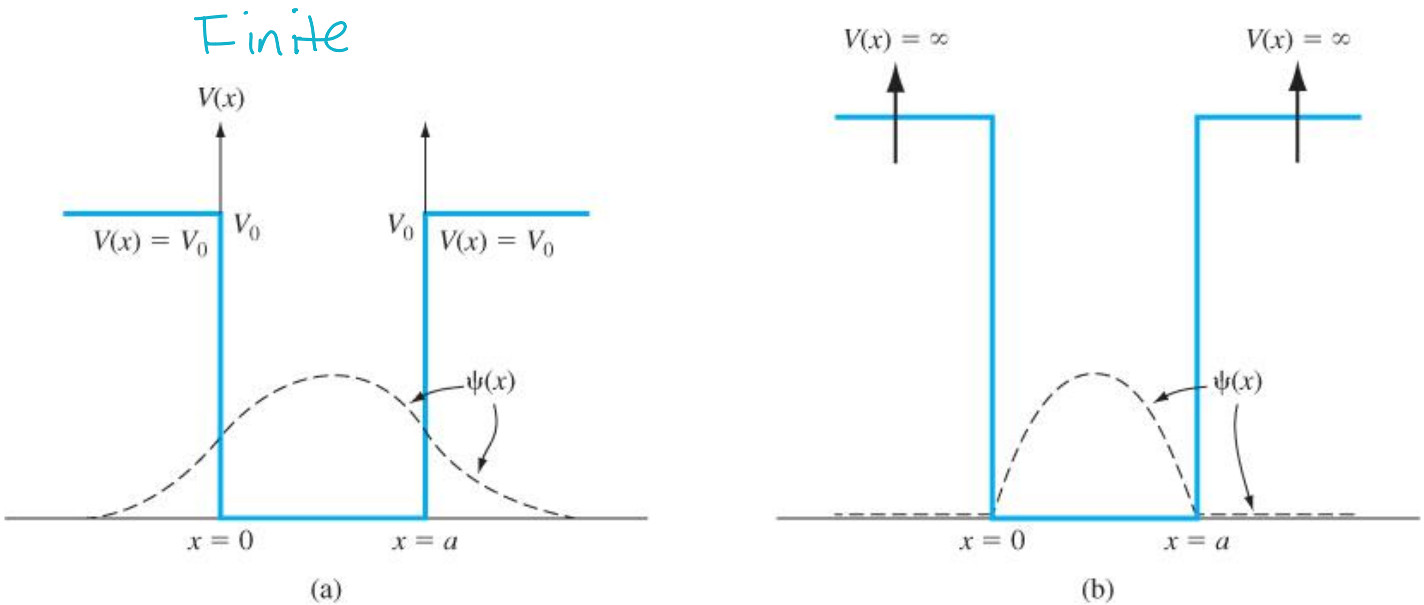


Figure 2.5 | Potential functions and corresponding wave function solutions for the case (a) when the potential function is finite everywhere and (b) when the potential function is infinite in some regions.

- Finite and infinite potential wells (bound particles) – energy quantized
- Potential height determines strength of confinement
- Solutions for $\psi(x)$ are sine and cosine functions for the infinite potential well

Infinite Potential Well – bound particle prbm "quantum well"

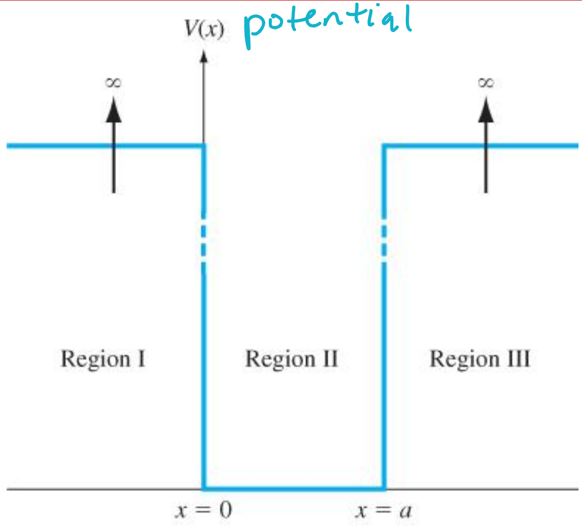


Figure 2.6 | Potential function of the infinite potential well.

Wave functions (eigen states):

$$\boxed{\psi(x) = \sqrt{\frac{2}{a}}\sin(k_n x)}$$

n is the quantum number

$$\boxed{k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{a}}$$

Quantized energy levels (eigen energies):

$$\boxed{E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}}$$

- Solution is a standing wave
- Total energy of the particle can only have discrete values (i.e., it is quantized) and it depends upon particle mass and well width
- Particle cannot have zero energy in this confined state
- Energies for electrons bound to atoms are also quantized

*see in-class derivation

Step 1: Schrodinger's Time Ind. Equation:

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

$\psi_{I} = 0$ $\psi_{III} = 0$

(particle not in I or III)

inside well $V(x) = 0$ $\therefore$

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - \cancelto{0}{V(x)})\psi(x) = 0$$

Soln: $\psi(x) = c_1 e^{jkx} + c_2 e^{-jkx}$

$= A_1 \cos(kx) + A_2 \sin(kx)$

Step 2: Apply boundary conditions

$\psi(0) = 0$, $\psi(a) = 0$

$\psi(0) = A_1 \longrightarrow A_1 = 0$

$\psi(x) = A_2 \sin(kx)$

then

$$\psi(a) = A_2 \sin(ka) = 0$$

↗ integer multiples of π

$ka = n\pi \qquad n = 1, 2, 3 \ldots$

(quantum #s)

↑

gives discrete energies $k = \frac{n\pi}{a}$

$$\psi(x) = A_2 \sin\left(\frac{n\pi}{a} x\right)$$

Step 3: Find A_2 using normalization of ψ

$$\int_{-a}^{a} |\psi(x)|^2 dx = 1$$

$$\int_0^a A_2^2 \sin^2\left(\frac{n\pi}{a} x\right) dx = 1$$

only eval. from $0 \to a$ b/c can't exist outside of well

$$A_2^2 \left| \frac{1}{2} x - \frac{1}{2} \cos\left(\frac{2n\pi}{a} x\right) \right.$$

angle identity

$$A_2 = \sqrt{\frac{2}{a}}$$

$$\therefore \quad \psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right)$$

Step 4: Calculate Energy

$$E = \frac{\hbar^2 k^2}{2m}$$

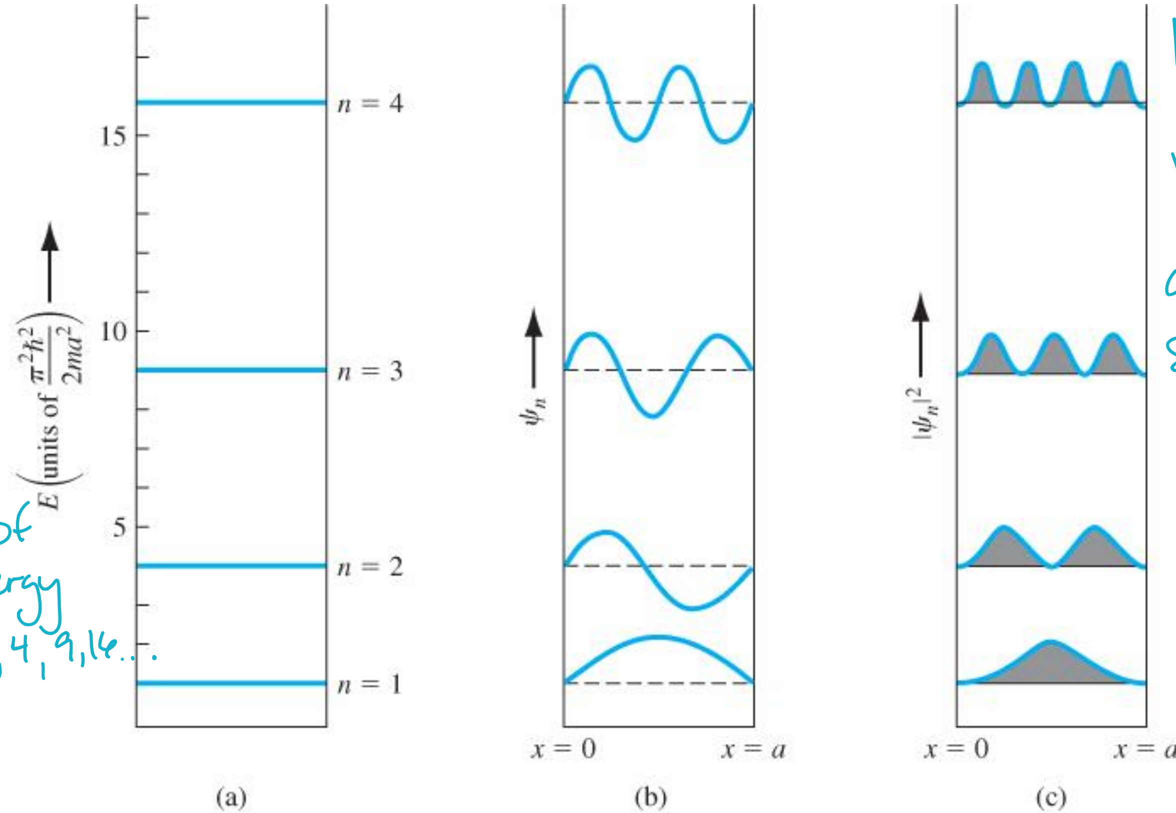
we know (see last lecture)

allowed discrete energy:

$$\frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

quantized energy levels based on #, mass, etc.

Infinite Potential Well



probability of particle being at some spot

because of n^2 → energy level is 1, 4, 9, 16...

Figure 2.7 | Particle in an infinite potential well: (a) four lowest discrete energy levels, (b) corresponding wave functions, and (c) corresponding probability functions. *(From Pierret [10].)*

If we know ground state and asked to find 5 level → multiple ground energy by 25.

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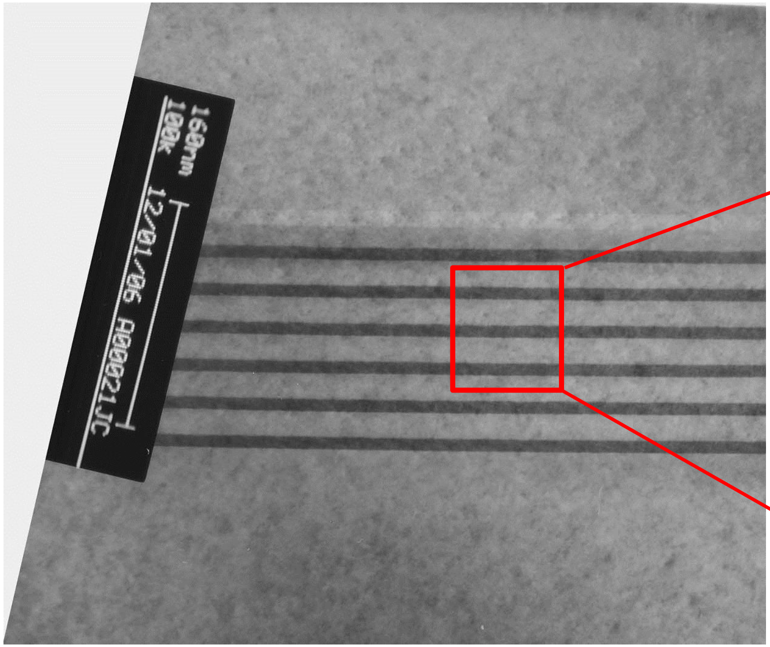
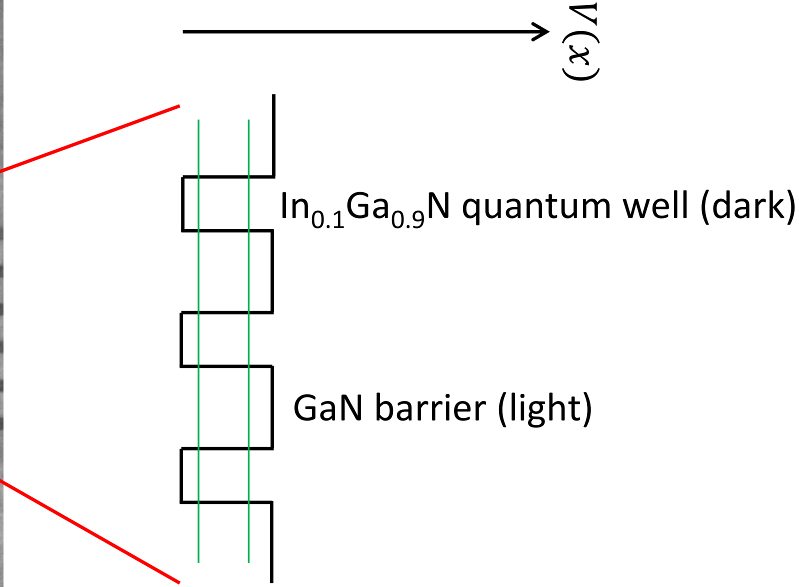
Real Potential Wells ("Quantum Wells")

- Real "quantum wells" are like potential wells with finite barriers
- The can be realized in semiconductors by alternating materials with different energy landscapes (energy bands)
- Electrons are confined and energy levels are quantized





High Electron Mobility Transistors (HEMTs)

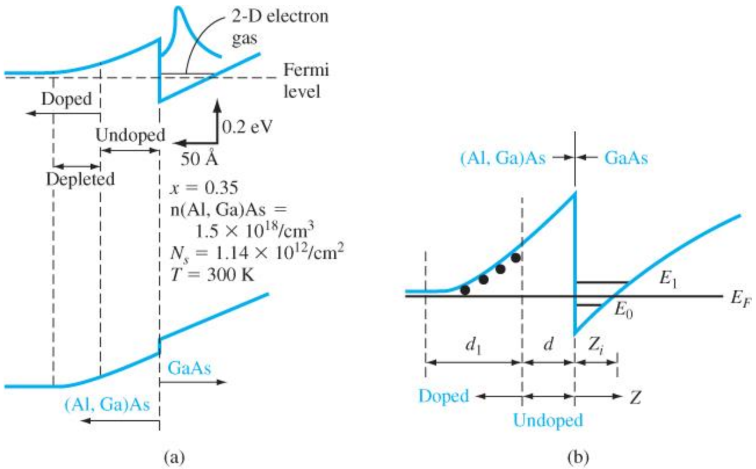


Figure 13.24 | Conduction-band edges for N-AlGaAs–undoped AlGaAs–undoped GaAs heterojunction.
(From Shur [13].)

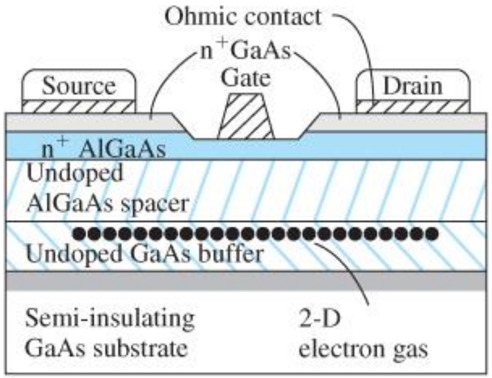


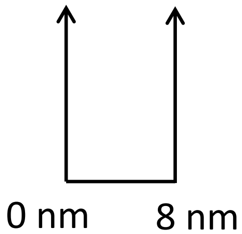
Figure 13.26 | A "normal" AlGaAs–GaAs HEMT.

2 different structures

- Quantum well formed at AlGaAs/GaAs heterostructure interface
- Separates carriers (electrons) from impurities (doping), reduces scattering, higher carrier velocity, higher switching frequency
- Transistor operates by conduction through the 2-D electron gas formed at the interface

Practice Questions

1. Calculate the second energy level (in eV) for an electron in an 8 nm wide infinite potential well
   – A: 2.35 eV
   – B: 0.0362 eV
   – C: 0.0059 eV
   – D: 0.0235 eV



2. If the particle is a proton instead of an electron, the energy level compared to the electron case will be
   – A: Higher
   – B: The same
   – C: Lower

3. What is the probability of finding the particle between 4 nm and 8 nm for a sinusoidal wave function (as in Fig. 2.7)
   – A: ½
   – B: 1
   – C: ¼
   – D: 0

(1.) $a = 8 \times 10^{-9}$ m

$\hbar = 1.054 \times 10^{-34}$

$m_e = 9.11 \times 10^{-31}$

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} = 3.765 \times 10^{-21} \text{ J}$$

$$\frac{3.765 \times 10^{-21} \text{ J}}{q} = 23.5 \text{ meV}$$

(2.) lower

(3.) $1/2$

alternatively integrate

$$\int_{a/2}^{a} |\psi(x)|^2 dx$$

Practice Questions

4. If a particle in a potential well has the following wave function (red lines, not realistic!), by what factor is the particle more likely to be found in the right side of the well than the left side

   – A: Equally likely

   – B: Twice as likely

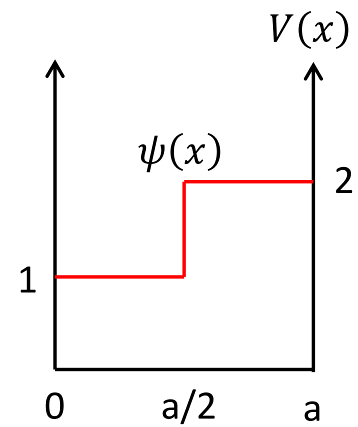
   – C: Four times as likely

   – D: Eight times as likely

prob. density = $|\psi|^2$

$\therefore$ 4x

$\psi(x) = 0$ outside



Step Potential Function

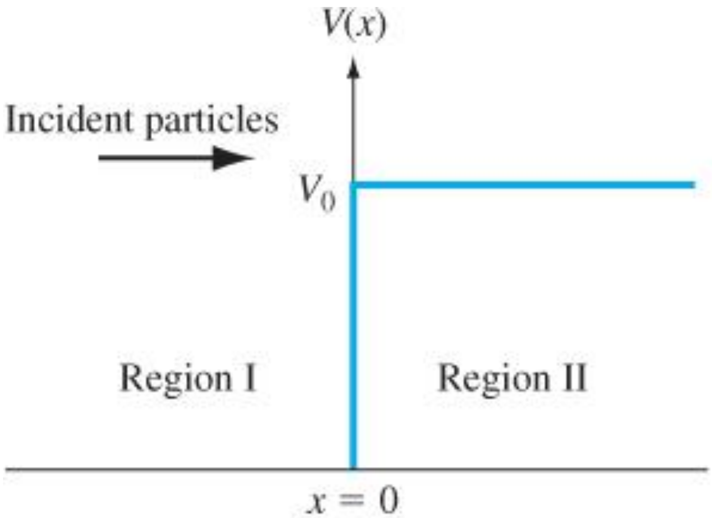


Figure 2.8 | The step potential function.

In region I the TISE is:

$$\boxed{\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0}$$

In region II the TISE is:

$$\boxed{\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\big(E - V(x)\big)\psi(x) = 0}$$

- Find solution in each region separately (for $E<V_0$)
- Match boundary conditions at x=0
- Derive reflection and transmission coefficients